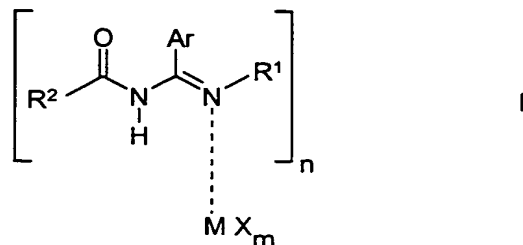


We claim:

1. An N'-substituted N-acylamidine-transition metal complex of the general formula I



where

M is a transition metal selected from the group of the metals Ni, Cu, Ru, Rh, Pd, Os, Ir and Pt

X is Cl, Br, triflate, methanesulfonate or p-toluenesulfonate

m is 0, 1 or 2,

n is 1, 2 or 3

and the radicals are defined as follows:

R<sup>1</sup>, R<sup>2</sup> are each a straight-chain, branched or cyclic hydrocarbon radical having from 1 to 20 carbon atoms which may be mono- or polyunsaturated, an aromatic radical having from 6 to 14 ring members which may be bonded directly or via a C<sub>1</sub>- to C<sub>6</sub>-alkyl or C<sub>2</sub>- to C<sub>6</sub>-alkylene group, and the radicals mentioned may bear one or more substituents selected from the group of C<sub>1</sub>- to C<sub>6</sub>-alkyl, C<sub>1</sub>- to C<sub>4</sub>-haloalkyl, OR<sup>3</sup>, NR<sup>4</sup>R<sup>5</sup>, COOR<sup>6</sup>, Si(R<sup>7</sup>)<sub>3</sub>, Si(R<sup>7</sup>)<sub>2</sub>R<sup>8</sup>, halogen, aryl, C<sub>3</sub>-C<sub>8</sub>-cycloalkyl,

R<sup>3</sup>, R<sup>6</sup>, R<sup>8</sup> are each independently C<sub>1</sub>- to C<sub>12</sub>-alkyl, C<sub>7</sub>- to C<sub>12</sub>-aralkyl, C<sub>6</sub>- to C<sub>10</sub>-aryl, C<sub>3</sub>- to C<sub>8</sub>-cycloalkyl, C<sub>3</sub>- to C<sub>8</sub>-cycloalkyl in which one CH<sub>2</sub> group has been replaced by O, NH or NR<sup>9</sup>,

R<sup>4</sup>, R<sup>5</sup>, R<sup>10</sup>, R<sup>11</sup> are each independently hydrogen, straight-chain or branched C<sub>1</sub>- to C<sub>12</sub>-alkyl, C<sub>7</sub>- to C<sub>12</sub>-aralkyl, C<sub>6</sub>- to C<sub>10</sub>-aryl, C<sub>3</sub>- to C<sub>8</sub>-cycloalkyl or C<sub>3</sub>- to C<sub>8</sub>-cycloalkyl in which one CH<sub>2</sub> group has been replaced by O, NH or NR<sup>9</sup>,

## 17

and  $R^4$  and  $R^5$  and/or  $R^{10}$  and  $R^{11}$  may each together be  $-(CH_2)_y-$ , where  $y$  is an integer from 4 to 7;

$R^7, R^9$  are each independently straight-chain or branched  $C_1-$  to  $C_{12}$ -alkyl or  $C_7-$  to  $C_{12}$ -aralkyl,

Ar is  $C_6$ - $C_{10}$ -aryl or hetaryl having from 5 to 10 ring members, and the radicals mentioned may be substituted by  $C_1-$  to  $C_6$ -alkyl,  $C_1-$  to  $C_4$ -haloalkyl,  $NR^{10}R^{11}$ ,  $COOR^6$ ,  $Si(R^7)_3$ ,  $Si(R^7)_2R^8$ ,  $OR^3$  and/or halogen.

2. A transition metal complex of the formula I as claimed in claim 1 where M is a transition metal selected from the group of Ru, Rh, Os, Ir, Pd and Pt.

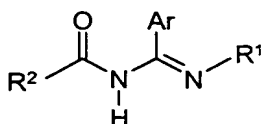
3. A transition metal complex of the formula I as claimed in claim 1 where M is Pd or Pt and m and n are each 2.

4. A transition metal complex of the formula I as claimed in any of claims 1 to 3 where

$R^1$  and  $R^2$  are each branched or unbranched  $C_1-$  to  $C_{12}$ -alkyl,  $C_7-$  to  $C_{12}$ -aralkyl,  $C_6-$  to  $C_{10}$ -aryl, and the radicals mentioned may be substituted by from one to three halogen atoms and/or one or two  $C_1$ - $C_6$ -alkyl, trifluoromethyl and/or  $C_1-$  to  $C_6$ -alkoxy substituents, and

Ar is  $C_6$ - $C_{10}$ -aryl or hetaryl having 5 or 6 ring members, and the radicals mentioned may be substituted by one or more  $C_1-$  to  $C_6$ -alkyl,  $C_1-$  to  $C_6$ -alkoxycarbonyl,  $C_1-$  to  $C_6$ -alkoxy, trialkylsilyl or diarylalkylsilyl and/or trifluoromethyl substituents and/or halogen.

5. A process for preparing N'-substituted N-acylamidine-transition metal complexes of the general formula I as claimed in any of claims 1 to 4, which comprises dissolving an N'-substituted N-acylamidine ligand of the formula III



III

and a transition metal compound containing the desired central atom M according to formula I in an organic solvent or in a mixture of different organic solvents and

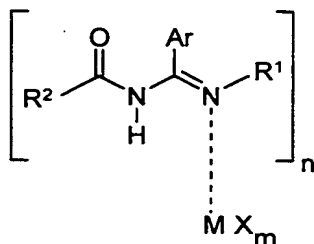
crystallizing the N'-substituted N-acylamidine-transition metal complex by adding a further solvent different to the solvent or solvent mixture used initially.

- 5      6. A process as claimed in claim 5, wherein the first solvent used is a halogenated or aromatic solvent or a mixture of different halogenated or aromatic solvents, and an ethereal solvent or solvent mixture is added for crystallization.
- 10      7. The use of an N'-substituted N-acylamidine-transition metal complex of the formula I as claimed in any of claims 1 to 4 as a catalyst.
8. The use as claimed in claim 7 for transition metal-catalyzed coupling reactions in which at least one new bond is formed between two carbon atoms.
- 15      9. The use as claimed in claims 7 and 8 for transition metal-catalyzed olefination, alkynylation, arylation or diaryl coupling reactions.

## N'-Substituted N-acylamidine-transition metal complexes and their use as catalysts

## Abstract

5 The present invention relates to N'-substituted N-acylamidine-transition metal complexes of the general formula I



10           where

M is a transition metal selected from the group of the metals Ni, Cu, Ru, Rh, Pd, Os, Ir and Pt

15        X        is Cl, Br, triflate, methanesulfonate or p-toluenesulfonate

$m$  is 0, 1 or 2,

**n** is 1, 2 or 3

and the radicals are defined as follows:

25  $R^1, R^2$  are each a straight-chain or branched, cyclic hydrocarbon radical having from 1 to 20 carbon atoms which may be mono- or polyunsaturated, an aromatic radical having from 3 to 6 ring members which may be bonded directly or via a  $C_1$ - to  $C_6$ -alkyl or  $C_2$ - to  $C_6$ -alkylene group, and the radicals mentioned may bear one or more substituents.

Ar is C<sub>6</sub>- to C<sub>10</sub>- aryl or hetaryl having from 5 to 10 ring members, and the radicals mentioned may be substituted by C<sub>1</sub>- to C<sub>6</sub>-alkyl, C<sub>1</sub>- to C<sub>4</sub>-haloalkyl, NR<sup>10</sup>R<sup>11</sup>, COOR<sup>6</sup>, Si(R<sup>7</sup>)<sub>3</sub>, Si(R<sup>7</sup>)<sub>2</sub>R<sup>8</sup>, OR<sup>3</sup> and/or halogen.

The invention further relates to a process for preparing this novel class of transition metal complexes and to their use as catalysts.